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NEWS 2 Apr 08 "Ask CAS" for self-help around the clock
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area
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NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available
NEWS 9 Jun 03 New e-mail delivery for search results now available
NEWS 10 Jun 10 MEDLINE Reload
NEWS 11 Jun 10 PCTFULL has been reloaded
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;
saved answer sets no longer valid
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY
NEWS 15 Jul 30 NETFIRST to be removed from STN
NEWS 16 Aug 08 CANCERLIT reload
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18 Aug 08 NTIS has been reloaded and enhanced
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
now available on STN
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced
NEWS 23 Sep 03 JAPIO has been reloaded and enhanced
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file
NEWS 25 Sep 16 Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 26 Sep 16 CA Section Thesaurus available in CAPLUS and CA
NEWS 27 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985
NEWS 28 Oct 21 EVENTLINE has been reloaded
NEWS 29 Oct 24 BEILSTEIN adds new search fields
NEWS 30 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 31 Oct 25 MEDLINE SDI run of October 8, 2002
NEWS 32 Nov 18 DKILIT has been renamed APOLLIT
NEWS 33 Nov 25 More calculated properties added to REGISTRY

NEWS EXPRESS October 14 CURRENT WINDOWS VERSION IS V6.01,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
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NEWS PHONE Direct Dial and Telecommunication Network Access to STN
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specific topic.

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FILE 'HOME' ENTERED AT 17:15:59 ON 01 DEC 2002

FILE 'REGISTRY' ENTERED AT 17:16:05 ON 01 DEC 2002
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 NOV 2002 HIGHEST RN 474744-87-1
DICTIONARY FILE UPDATES: 29 NOV 2002 HIGHEST RN 474744-87-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

```
=> s 4-bromo-2-methoxyestradiol
      11862466 4
      938248 BROMO
      14553906 2
      22 METHOXYESTRADIOL
L1      1 4-BROMO-2-METHOXYESTRADIOL
      (4 (W) BROMO (W) 2 (W) METHOXYESTRADIOL)
```

=> file caplus
COST IN U.S. DOLLARS
SINCE FILE ENTRY TOTAL
SESSION
FULL ESTIMATED COST 16.38 16.59

FILE 'CAPLUS' ENTERED AT 17:16:38 ON 01 DEC 2002
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FILE COVERS 1907 - 1 Dec 2002 VOL 137 ISS 23
FILE LAST UPDATED: 29 Nov 2002 (20021129/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> d 11 ibib hitstr abs
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG	- RN
SAM	- Index Name, MF, and structure - no RN
FIDE	- All substance data, except sequence data
IDE	- FIDE, but only 50 names
SQIDE	- IDE, plus sequence data
SQIDE3	- Same as SQIDE, but 3-letter amino acid codes are used
SQD	- Protein sequence data, includes RN
SQD3	- Same as SQD, but 3-letter amino acid codes are used
SQN	- Protein sequence name information, includes RN
CALC	- Table of calculated properties
EPROP	- Table of experimental properties
PROP	- EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract

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APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS --ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):end

=> d 11 ibib hitstr abs
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:N

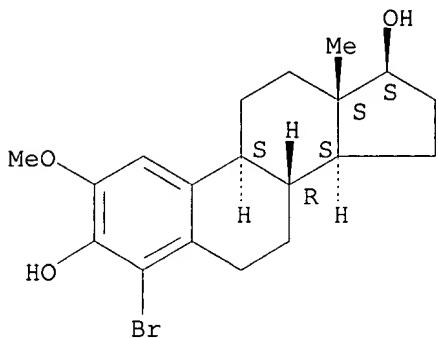
=> s 11
L2 2 L1

=> d 12 1-2 ibib hitstr abs

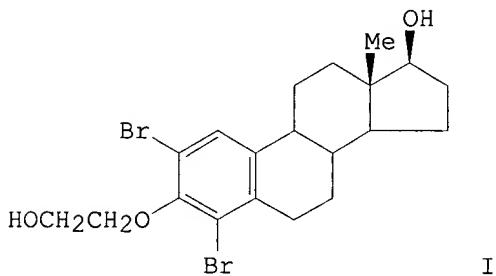
L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:633338 CAPLUS
DOCUMENT NUMBER: 111:233338
TITLE: Preparations of 2,4-disubstituted estradiols
AUTHOR(S): Pert, Derek J.; Ridley, Damon D.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Sydney, Sydney, 2006, Australia
SOURCE: Australian Journal of Chemistry (1989), 42(3), 421-32
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:233338
IT 97515-50-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 97515-50-9 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 4-bromo-2-methoxy-, (17.beta.)- (9CI)
(CA INDEX NAME)

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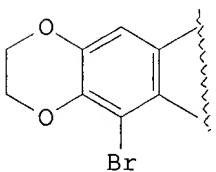
Absolute stereochemistry.



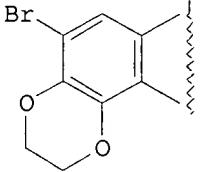
GI



I



II



III

AB Dibromoestradiol I was treated with CuCl₂/NaOMe to give [2,3]dioxane II as the major product as well as a minor amt. of the [3,4]dioxane deriv. III. The compds. were used to prep. a no. of 2,4-disubstituted estradiol derivs. Alternative routes to other 2,4-disubstituted estradiols are described.

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:465176 CAPLUS

DOCUMENT NUMBER: 103:65176

TITLE: Catechol formation of fluoro- and bromo-substituted estradiols by hamster liver microsomes. Evidence for dehalogenation

AUTHOR(S): Li, Jonathan J.; Purdy, Robert H.; Appelman, Evan H.; Klicka, John K.; Li, Sara Antonia

CORPORATE SOURCE: Med. Res. Lab., Veterans Adm. Med. Cent., Minneapolis, MN, 55417, USA

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SOURCE: Molecular Pharmacology (1985), 27(5), 559-65
CODEN: MOPMA3; ISSN: 0026-895X

DOCUMENT TYPE: Journal
LANGUAGE: English

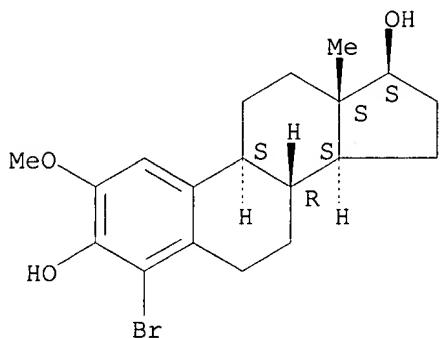
IT 97515-50-9

RL: FORM (Formation, nonpreparative)
(formation of, from halogenated estrogens by liver microsome)

RN 97515-50-9 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 4-bromo-2-methoxy-, (17.beta.)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



AB Liver microsomes from castrated hamsters were incubated with 2-fluoro-, 4-fluoro-, or 2,4-difluoroestradiols and analogous bromo-substituted estradiols to det. the extent of 2- and 4-hydroxylation with these substrates. Estrogen 2-hydroxylase [9055-96-3] and estrogen 4-hydroxylase [80237-93-0] activity was detd. by radioenzymic assay, and the 3H-labeled monomethyl ether products were identified by HPLC. With unsubstituted 17beta.-estradiol [50-28-2] as substrate, 97% of the product formed was 2-hydroxylated, and 3% was 4-hydroxylated. The monosubstituted fluoroestradiols exhibited >2-fold enhanced ability to form catechol estrogens compared with their corresponding bromoestradiols. Data presented indicated substantial defluorination when 2-fluoroestradiol [16205-32-6] was the substrate, which amounted to 36% of the total product formed, and 32% of the rate of 2-hydroxylation found with unsubstituted 17beta.-estradiol as substrate. Interestingly, the rate of 4-hydroxylation was elevated 20- and 6.7-fold, resp., when 2-fluoroestradiol and 2,4-difluoroestradiol [97515-43-0] were the substrates compared to the rate with 17beta.-estradiol. Moreover, both 4-fluoroestradiol [1881-37-4] and 2,4-difluoroestradiol exhibited at least a 1.6-fold greater rate of 2-hydroxylation compared with 17beta.-estradiol. In contrast, the rate of dehalogenation with 2-bromoestradiol [15833-07-5] was only 12% of that found with 2-fluoroestradiol. No debromination was obtained with 4-bromoestradiol [1630-83-7] and essentially no catechols were formed using 2,4-dibromoestradiol [19590-55-7] as substrate with these hamster liver microsomes. These data provide evidence for defluorination of these substituted estrogens, particularly at the C-2 position, and seriously hamper the use of fluoroestrogens in studies of hormonal carcinogenicity.